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Abstract: We consider a collocation method using radial functions for the solution of partial differential equations in irregular domains. We use a regularised least squares approach to solve the potentially ill-conditioned problems that may arise. This meshless method is easy to implement and eliminates most of the problems that mesh oriented methods have with irregular boundaries and complicated domains. When solving, also, for the position and shape parameters of the radial functions we obtain an adaptive, albeit non-linear, method. In this case, the resulting problem is a separable non-linear least squares one that can be efficiently solved by the Variable Projection method.

Keywords: elliptic problems; collocation; meshless; TSVD; variable projections; radial functions.

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1 Introduction

Radial basis function collocation methods for solving partial differential equations are truly meshfree algorithms, in the sense that collocation points can be chosen freely and no connectivity between the points is needed or used (Kansa, 1990a, 1990b; Narcowich et al., 1994). These methods, which are spatial dimension independent, can be easily extended to solve 3D problems. Moreover, due to the absence of a grid, these techniques are better suited than classical methods to cope with problems having complex boundaries.

On the other hand, despite the advances of the last decade, there are many open problems, both from a theoretical and a numerical point of view. To mention some of them:

- The invertibility of the algebraic system of equations corresponding to the asymmetric collocation method is still a conjecture (Hon and Schaback, 2001).
- From a numerical point of view, it is well known (Schaback, 1995) that the increase in the number of basis functions produces an increase in the condition number of the corresponding collocation matrix. Except for pre-conditioning techniques this problem is extant.

The methods described in this paper deal with these two issues by using regularised least squares calculations, which are robust under high levels of ill-conditioning. We also offer a new global error estimation procedure and two types of nodal basis adaptation.

The collocation methods to be considered are based on the interpolation theory of radial basis functions and can be classified according to the different kernels associated with these techniques.

Let $\phi: R^+ \rightarrow R$; $R(\mathbf{x}) = \phi(\|\mathbf{x} - \mathbf{x}^*\|)$, where $\|\cdot\|$ is the Euclidean norm in R^n ; then, if we let $\{\mathbf{x}_i^*\}_{i=1}^{\beta} \subset D \subset R^n$, the RBF interpolation problem is defined by

$$y(\mathbf{x}) = \sum_{i=1}^{\beta} w_i R(c_i, \mathbf{x} - \mathbf{x}_i^*) + p(\mathbf{x}), \quad y(\mathbf{x}_j) = y_j, \quad j = 1, \dots, \kappa,$$

$x \in R^n$ where $\{x_j, y_j\}_{j=1}^k$ are data pairs. In the former equation, c_i , is called the *shape parameter*, and $p \in P^l(R^n)$ (the polynomials of degree l in R^n), depend on the specific RBF R .

These kernels can be broadly divided into three groups: the piecewise kernels, the C^∞ radial functions and compact support radial basis functions. The most representative examples of these groups are, respectively: the thin plate splines (Duchon, 1977), the Wendland (1995) and Wu (1995) compact support RBF and the C^∞ multi-quadric and Gaussian kernels. For C^∞ radial basis functions it has been proved that spectral order of convergence holds depending both on the fill distance and the shape parameter c_i (Buhmann, 2003). However, the requirement of good conditioning is at odds with the accuracy of the interpolation, the so called problem of “good conditioning vs. good fit”.

Preconditioning techniques, (Beatson et al., 1999; Ling and Kansa, 2004), domain decomposition algorithms (Hon and Wu, 2000; Li and Hon, 2004; Muñoz-Gomez et al., 2006b; Zhou et al., 2003) and node adaptive strategies, which we shall mention below, have appeared in the literature to deal with this problem. In the field of node adaptive methods, several algorithms have been published. In Behrens and Iske (2002) and Behrens et al. (2001), one of the authors has formulated an adaptive strategy based on local RBF interpolants in two dimensions. This technique has been successfully applied, in a semi-Lagrangian context, to linear evolutionary PDEs.

In Wu (2004, 2005) an adaptive meshfree RBF algorithm for non-linear scalar conservation laws was developed and successfully applied to the inviscid Burger equation. Although this method is formulated in one dimension, the author points out how to extend his technique to two dimensions.

Other techniques (Hon, 1999; Sarra, 2005; Schaback, 1995), mainly in one dimension, have been also developed for different RBFs. More recently, in (Muñoz-Gomez et al., 2006a), an adaptive node scheme based on thin plate spline kernels is developed by using local error estimates combined with a quad-tree type algorithm. Moreover in Driscoll and Heryudono (2006), the authors built an adaptive algorithm based on multi-quadric kernels, in which both the nodes and the shape parameters are adapted. Their results are applied to linear and non-linear problems in two space dimensions.

In all these algorithms the centres and the collocation points coincide. The case when this is not so has been barely treated in the literature. As it has been pointed out in Fasshauer (2005), “*There are only limited results addressing the situation in which the centres for the basis functions and the data sites may differ*”. Among the few results related to this problem, we have those in Quak et al. (1993) and Sivakumar and Ward (1993), where the authors deal with discrete and continuous least squares approximation problems, respectively. In both papers the authors investigate the non-singularity of the coefficient matrix obtained from a system of normal equations. However, these works do not investigate the collocation techniques for PDE. Thus, some of the results presented in this paper pertain to a fairly new area of research.

In Pereyra and Scherer (2006), some of us have demonstrated the use of tensor product B-spline bases to solve elliptic problems in 2 and 3 dimensions on irregular domains, using embedding and an overdetermined system of collocation points. The key there was to employ regularised linear least squares methods to solve the resulting algebraic problem, since the scattered collocation points on the non-rectangular domain could easily lead to ill-conditioned, or even rank deficient, problems. In that and previous

works on scattered data fitting (Pereyra and Scherer, 2002a; 2002b), we used effectively truncated SVD's and conjugate gradients as possible approaches to solve those ill-posed linear least squares problems.

We will do likewise here in the case that no adaptive radial basis functions are used. The additional novelty in this work is in the use of radial functions and adaptive bases based on the solution of a separable non-linear least squares problems by the Variable Projection method.

The key concept in that method is to solve analytically for the linear weights, leading to the Variable Projection functional containing only the non-linear parameters, which is then solved by any conventional procedure for non-linear least squares, such as Marquardt's or its variations. This method has been extremely effective through the years for fitting linear combinations of exponentials, Gaussians and many other types of non-linear functions to data, as is documented in Golub and Pereyra (2003).

We also implement a global error estimation algorithm that is akin to a deferred correction approach and use it as a monitor function in an additional refinement post-process, based on error equidistribution, in order to achieve a desired accuracy.

2 Elliptic problems

2.1 Problem formulation and discretisation by collocation

Given an elliptic partial differential equation

$$F(y(\mathbf{x})) = 0, \quad \mathbf{x} \in D \subset R^n,$$

with boundary conditions

$$B(y(\mathbf{x})) = 0, \quad \mathbf{x} \in \partial D, \quad (1)$$

we consider the Ansatz

$$y(\mathbf{x}) = \sum_{i=1}^{\beta} w_i R(c_i; \mathbf{x} - \mathbf{x}_i^*), \quad (2)$$

where the R 's are radial functions, c_i is the *shape parameter* and $\{\mathbf{x}_i^*\}$ is the *centre point*.

In the case of Gaussian basis functions we have:

$$R(c_i; \mathbf{x} - \mathbf{x}_i^*) = G(c_i; \mathbf{x} - \mathbf{x}_i^*) = e^{-c_i^2 \|\mathbf{x} - \mathbf{x}_i^*\|^2}.$$

The Ansatz is then replaced in the differential equations and boundary conditions and a number κ of collocation points X_k , equal or larger than the number of free parameters, are chosen. We finally obtain the discrete problem to be solved in order to approximate the exact solution:

$$F\left(\sum_{i=1}^{\beta} w_i R(c_i; \mathbf{x}_k - \mathbf{x}_i^*)\right) = 0, \quad \mathbf{x}_k \in D,$$

$$B\left(\sum_{i=1}^{\beta} w_i R(c_i; \mathbf{x}_k - \mathbf{x}_i^*)\right) = 0, \quad \mathbf{x}_k \in \partial D. \quad (3)$$

If we prescribe the non-linear parameters c_i, \mathbf{x}_i^* , then this is either a square ($\beta = \kappa$) or an overdetermined linear system ($\beta < \kappa$). The most common case is the first, which then requires a linear equation solver. In the less common second case, we can only minimise the residual if we use the two-norm that lead to a linear least squares problem. We emphasise that the collocation points need not be coincident with the centres of the basis functions.

If the parameters of the radial functions are not prescribed but are also to be determined, then it is necessary to select enough collocation points to account for these additional degrees of freedom. The problem now is non-linear and it requires appropriate techniques.

Clearly, in order to activate the boundary conditions, collocation points and/or basis function centres should be selected both in the interior as well as in the boundary of the domain. In principle, there is no impediment to having basis function centres in the exterior of the domain.

Observe that, in this somewhat abstract presentation, the boundary conditions can be as general as desired and also the order of the differential operator can be arbitrary. We only assume that the problem is well posed and has a unique solution. As a matter of fact, F and/or B could also be non-linear or time dependent, although we do not discuss those cases in this paper.

Observe also that, since there is no mesh connecting either the basis functions or the collocation points, there are no special problems with the discretisation near the boundaries. The boundaries (either exterior or interior) need to be identified in the formulation of the problem, in order to know how to select points on them or in the interior of the integration domain and also to apply the appropriate collocation conditions.

Depending on the distribution of collocation points and the position of the basis function centres the discrete system can be ill-conditioned, for instance, if for some radial basis function there are not enough collocation points within its effective support.

3 Global error estimation and basis equidistribution

Let $u(\mathbf{x})$ be the exact solution of the linear BVP (1) and let $y(\mathbf{x})$ be the collocation approximation. Then, the global error $e(\mathbf{x}) = u(\mathbf{x}) - y(\mathbf{x})$ satisfies:

$$\begin{aligned} F(e(\mathbf{x}_j)) &= -r(\mathbf{x}_j), \\ B(e(\mathbf{x}_i)) &= -rb(\mathbf{x}_i), \end{aligned} \quad (4)$$

where $r(\mathbf{x}) = F(y(\mathbf{x}))$ and $rb(\mathbf{x}) = B(y(\mathbf{x}))$ are the residuals evaluated at (possibly) a different set of control points. This is done since, in the interpolation case, those residuals would be essentially zero, if they were evaluated at the same points for which the weights were obtained; in this way we also monitor the approximate solution elsewhere, a more reliable and significant test.

Thus, solving equation (4), where $e(\mathbf{x})$ is replaced by a linear combination of the same basis functions used earlier with weights w_e , we can obtain an approximation to the global error *everywhere* in the domain. This is quite different from the ‘local error’ estimates commonly used (Behrens et al., 2001) and it is more of the classical deferred correction type (see Driscoll and Heryudono, 2006; Pereyra, 1984). Although it is not a rigorous estimate (and certainly not a bound), it gives additional (hopefully useful) information on the numerical solution obtained by this method in real life problems.

Observe that for linear differential equations, even in the adaptive case, only a linear least squares solve is required to obtain the weights of the collocation solution $e(\mathbf{x})$. In consequence, this process amounts to a correction of the weights:

$$w_i^{(2)} = w_i + w_e e_i.$$

We can use this global error estimate as a monitor function in a post-process to approximately equidistribute the error, by adding $k - 1$ ($k > 1$) basis functions where the error is greater than k times the average. Naturally, this solve-error estimate-add basis functions process can be re-iterated, such as is done in Driscoll and Heryudono (2006), where the residual is used as the monitor error function.

3.1 Example: Poisson’s equation in 2D

We exemplify the above procedure in a simple case: Poisson’s equation with Dirichlet boundary conditions on a general domain $D \subset R^2$:

$$\Delta y(\mathbf{x}) = g(\mathbf{x}), \quad \mathbf{x} \in D,$$

$$y(\mathbf{x}) = b(\mathbf{x}), \quad \mathbf{x} \in \partial D.$$

We choose Gaussians for our basis functions and consider first the general case with fixed parameters c_i, \mathbf{x}_i^* . In order to apply the differential operator to the Ansatz we need the second partial derivatives of the Gaussians:

$$\frac{\partial^2 G}{\partial x_l^2} = 2c^2 G [2c^2 (x_l - x_l^*)^2 - 1], \quad l = 1, 2.$$

The linear least square problem takes the form (with appropriate additional equations for the boundary collocation points):

$$\min_w \sum_{k=1}^{\kappa} \left\{ 4 \sum_{l=1}^{\beta} w_l \left\{ c_l^2 G_l(c_l; \mathbf{x}_k - \mathbf{x}_l^*) \left[\sum_{l=1}^2 c_l (x_{kl} - x_{ll}^*)^2 - 1 \right] \right\} - g(\mathbf{x}_k) \right\}^2,$$

while for the non-linear adaptive one the minimisation is on all the parameters $[\mathbf{w}; \mathbf{c}; \mathbf{x}^*]$

When determining the non-linear parameters we will also need the partial derivatives of G with respect to them:

$$\frac{\partial G}{\partial c} = -2cG(\mathbf{x} - \mathbf{x}^*)^2, \quad \frac{\partial G}{\partial \mathbf{x}_l^*} = 2c^2 G(x_l - x_l^*), \quad l = 1, 2.$$

3.2 Numerical examples for Poisson's equation in 2D

We consider the problem of subsection 3.1 for:

$$g(\mathbf{x}) = -25(\sin(5x_1) + \sin(5x_2)); \quad b(\mathbf{x}) = \sin(5x_1) + \sin(5x_2),$$

with D being a circle of radius 1 embedded in the unit square. We consider first a uniform mesh of 20×20 points in the unit square that results in 276 collocation points in the circle's interior. We also take 180 points in the boundary of D , equally spaced at 2° . The basis functions centres are the same as the interior collocation points, while the shape parameter $c = 1.0$.

We use a truncated SVD algorithm to solve the resulting $456 \times \text{rank}$ problem. This results in an effective regularisation procedure, as we see in Table 1. The value of $\text{rank} \leq 276$ is determined by the threshold used to cut the small singular values that are the source of ill-conditioning.

Table 1 Results for Poisson's equation and various TSVD thresholds

<i>Maximum error</i>	<i>Estimated error</i>	<i>TSVD threshold</i>	<i>Rank</i>	<i>Condition</i>
0.0001	0.000012	10^{-12}	55	72×10^{10}
0.0012	0.00032	10^{-10}	45	88×10^8
0.013	0.017	10^{-8}	32	80×10^6
0.066	0.028	10^{-6}	21	34×10^5

Next, we allow also basis functions in the boundary and finally we choose the interior collocation points and the interior basis function centres and shape parameters at random. The best results are shown in Table 2. Here, $(20 \times 20) + 360 : 636$, means that 276 points were chosen in the interior of D from a uniform (20×20) mesh in the unit square and 360 points were chosen uniformly distributed in the boundary, for a total of 636 points. (R) indicates that the points in the interior of the domain were taken at random, while in the c column (R) means that the values of c were taken at random in the indicated interval. We also include a couple of runs with the node adaptive procedure of Section 4.

Table 2 Best results for various modalities

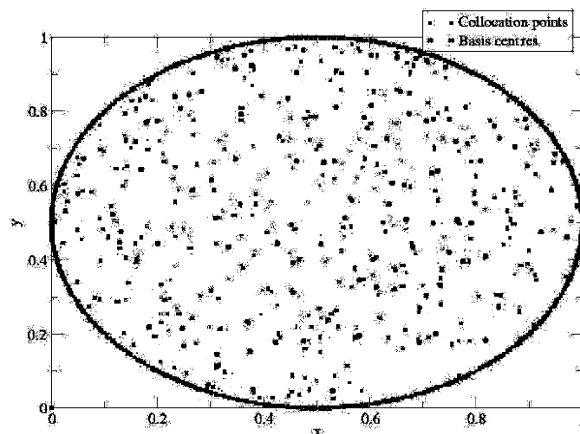
<i># coll.</i>	<i># basis</i>	<i>Max. error</i>	<i>Est. error</i>	<i>Rank</i>	<i>c</i>	<i>Time</i>
400 + 360 : 636	400 + 360 : 636	0.0086	0.011	32	1.0	1.11''
400 + 360 : 636	400 + 360 : 636	0.0030	0.0014	68	2.0	9.44''
301 R + 360 : 661	301 R + 360 : 661	0.00020	0.000026	79	[0.5, 2.0] R	12.52''
225 + 60 : 205	15 : Adaptive	0.0044	0.0023	—	—	10.3''
205	30 : Adaptive	0.000047	0.00015	—	—	33.8''
205	45 : Adaptive	0.0000016	0.00008	—	—	74.6''

The computing times (in seconds) correspond to an Opteron 2.4 GH PC under LINUX; the implementation uses FORTRAN 95 with the INTEL ifort compiler. The threshold was in all cases 10^{-8} . For the adaptive case we started from ten different sets of random initial values for the non-linear parameters ($3 \times \#basis$). We report the

best results and the average computational time. We show the effects on accuracy and computing times due to the increase in the number of basis functions.

In Figure 1 we see the distribution of collocation and basis centres for the random choice above (third test).

Figure 1 Distribution of randomly chosen points



The second example is from Driscoll and Heryudono (2006). It is also Poisson's equation, now in the square $[-1, 1]^2$, with

$$g(x_1, x_2) = 40(10(x_1^2 + x_2^2) - 1) R(x_1, x_2),$$

$$b(x_1, x_2) = R(x_1, x_2), \quad R(x_1, x_2) = e^{-10(x_1^2 + x_2^2)}. \quad (5)$$

The solution is $R(x_1, x_2)$ and therefore the problem is trivial for collocation with Gaussians, if we assume the correct shape parameter $c^2 = 10$. In fact, for a very small 3×3 nodal set, with a basis function at $(0, 0)$ we get very good accuracy as expected. The weight for the central basis function is 1 and those for the boundary ones are essentially zero. Accuracy is very good for various numbers of uniformly placed nodes. Also, if we set the shape parameter to other values we can still get some reasonable results, until we get too far from the correct value. A summary of results is shown in Table 3 and more on this problem using an adaptive procedure can be found in Section 5.

Table 3 Results for example 2

$N_{coll.}$	$N_{bas.}$	$Thresh$	$Max. error$	$Est. error$	$Rank$	c^2	$Time$
64 + 20	9	10^{-10}	8.3×10^{-11}	4.5×10^{-13}	9	10	0.012''
25 + 40	25 + 40	10^{-10}	1.2×10^{-10}	2.9×10^{-11}	49	10	0.016''
400 + 160	400 + 160	10^{-10}	7.8×10^{-8}	1.4×10^{-6}	293	10	4.93''
100 + 40	100 + 40	10^{-10}	0.0082	0.12	104	8	0.08''
400 + 80	400 + 80	10^{-10}	8.1×10^{-7}	1.7×10^{-5}	246	8	5.06''
400 + 80	400 + 80	10^{-10}	1.2×10^{-4}	6.4×10^{-5}	171	5	2.95''

Driscoll and Heryudono report a maximum error of 4.54×10^{-5} , using 260 multi-quadrics, $\phi(x_1, x_2) = \sqrt{1 + \varepsilon^2(x_1^2 + x_2^2)}$ and a node adaptation algorithm that took four iterations to settle down.

4 Direct node adaptation

The conventional approach to nodal adaptation (see Section 3 and Babuska (1976), Behrens et al. (2001), Behrens (2005), Pereyra and Sewell (1975) Muñoz-Gomez et al. (2006a) and Hon and Wu (2005)) relies on a multi-pass approach. An initial nodal set for the basis functions is chosen, the collocation problem is solved, some kind of (usually local) error estimation is obtained from the initial approximate solution and a refinement or relocation of the nodes is effected. This procedure can then be re-iterated.

We propose to explore a variation on this approach in which, instead of using an arbitrary initial set of nodes, we solve the collocation equations, possibly on a coarse set, both for the weights w and for the location \mathbf{x}^* and shape parameters c of the basis functions. The collocation equations become then a separable non-linear least squares problem that is amenable to solution by the Variable Projection method (Golub and Pereyra, 1973, 2003).

We can combine both approaches by using the global estimation of Section 3 in order to introduce further basis functions where the errors are not approximately equidistributed or if the desired accuracy has not been reached.

As an illustration we consider the collocation procedure for Poisson's equation, discussed in Section 3.1. The least squares problem 3.1 is now non-linear and separable. If we write it in matrix form:

$$\min_{\mathbf{w}, \mathbf{c}, \mathbf{x}^*} \|\Gamma(\mathbf{c}, \mathbf{x}^*) \mathbf{w} - \phi\|_2^2,$$

where ϕ represents the right hand side, then, for each set of fixed values of \mathbf{c} , \mathbf{x}^* , the linear parameters \mathbf{w} can be eliminated by solving (analytically) the corresponding linear least squares problem as:

$$\mathbf{w} = \Gamma^+ \phi,$$

where Γ^+ is the pseudoinverse of the matrix Γ . Replacing this expression we obtain the reduced Variable Projection functional, with minimisation now only required on the nonlinear parameters:

$$\min_{\mathbf{c}, \mathbf{x}^*} \|(\Gamma(\mathbf{c}, \mathbf{x}^*) \Gamma^+(\mathbf{c}, \mathbf{x}^*) - I)\phi\|_2^2.$$

This problem can be solved by using VARPRO, the algorithm developed in Golub and Pereyra (1973). A good modern public implementation can be found in Gay (2002).

5 Numerical examples of node adaptation

We revisit Poisson's equation (5) from Driscoll and Heryudono (2006), but now we allow the parameters of the Gaussians to vary, starting from ten random initial values

and using VARPRO to solve the resulting separable non-linear least squares problem. We take 8×8 points in the interior and 20 collocation points in the boundary of the domain. The maximum error is reported on an uniform 11×11 mesh. The calculation was performed in double precision. Only three of the ten trials were successful, returning $(\sqrt{10}, 0, 0)$ to full double precision accuracy, with the error estimation and VARPRO termination flags giving a clear indication of failure or success. Thus, a first lesson learned is that when this non-linear multi-modal estimation problem is solved with a locally convergent algorithm, such as VARPRO, it is necessary to add some kind of global optimisation approach in order to better explore the input space for appropriate solutions, as we have done by trying multiple initial values.

Now we consider a more complicated domain, limited by the astroid curve:

$$(x_1^2 + x_2^2 - 1)^3 + 27x_1^2x_2^2 \leq 0.$$

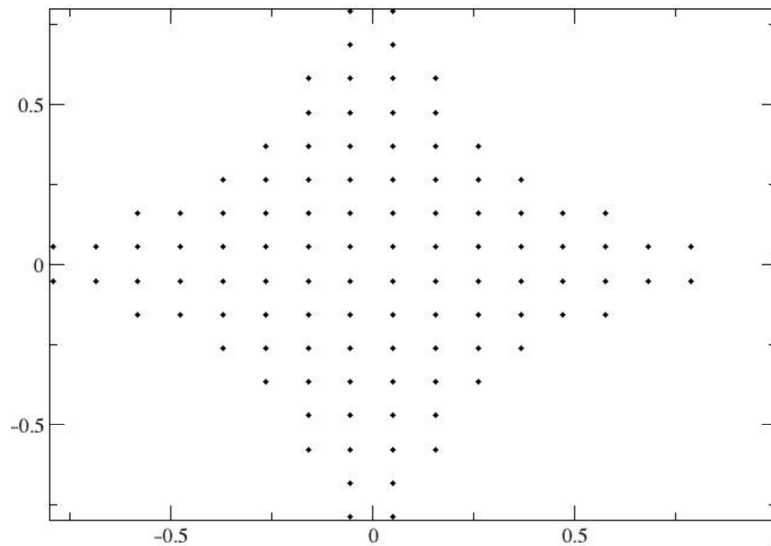
We use a 20×20 uniform mesh in the unit square and select the 108 points that fall in the interior of the domain. We also take 40 points on the boundary at equally spaced angles, using the parametric form of the astroid (see Figure 2):

$$x_1 = \cos^3 \theta,$$

$$x_2 = \sin^3 \theta.$$

We consider three Gaussians and determine their parameters from randomly generated initial values. Invariably, the algorithm picks the correct Gaussian and generates linear weights that are essentially $(\sqrt{10}, 0, 0)$. The accuracy is full double precision, of course, and the error estimator is very accurate.

Figure 2 Poisson's equation inside an astroid collocation points



For the next problem we consider an L-shaped membrane with the same equation, number of basis functions and collocation points as in the previous problem. The results are entirely similar.

We finally consider another problem from Driscoll and Heryudono (2006). The domain is the same L-shape as above, but now we use the forcing function

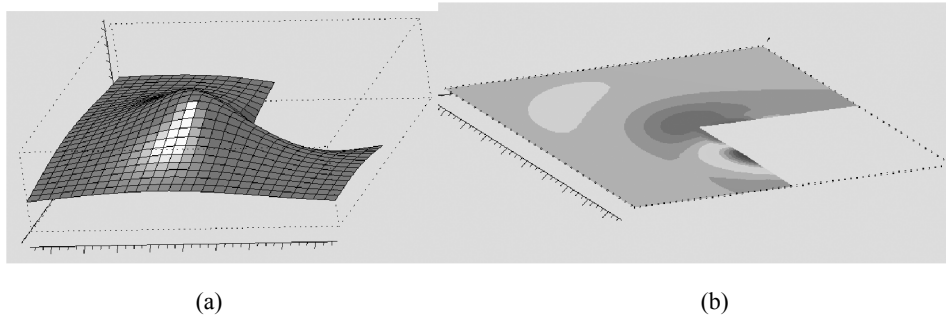
$$g(\mathbf{x}) = -10e^{-10(x_1-0.1)^2+(x_2-0.1)^2}$$

and 0 boundary conditions, resulting in a problem with no analytic solution and a re-entrant corner singularity. We use a 30×30 uniform mesh in the interior, 120 collocation points on the boundary and ten basis functions chosen at random in $[0, 0.2] \times [0, 0.2]$, with the shape parameters in the interval $[3, 3, 3]$ (see Figure 4). After ten trials the best results have a maximum estimated error of 0.00068. The VARPRO results for that best run show a residual of 0.093 with a maximum gradient component of 2.2×10^{-7} . The average time per run was 11.3".

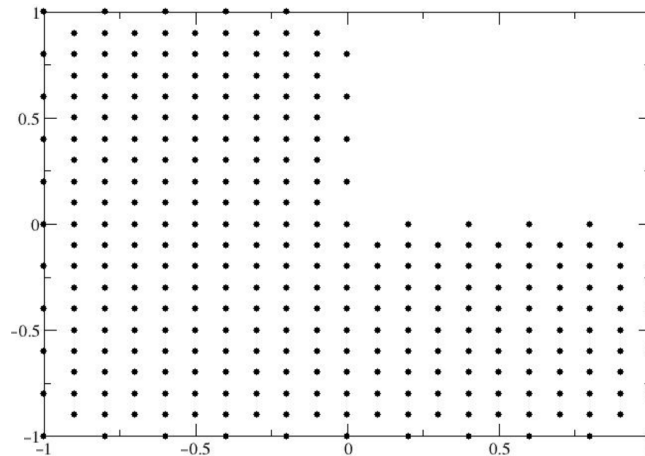
One question to ask would be: is it necessary to make multiple runs? Besides avoiding the possibility of failure, we can report that the best run (from random initial values) was not the first one, which had an estimated error of 0.001; so the added expenditure of running ten times improves the reliability and the accuracy by a significant factor.

Subsequently, after each trial and by using the global error estimation as a monitor function, we approximately equidistribute the error by introducing k new nodes where the error is k times larger than the average. We limit the refinement to adding at most 50% more nodes at a time. In one first pass, which brings the number of basis functions to 15, we obtain a maximum estimated error of 0.00018, for an almost fourfold accuracy improvement. We observe that these nodes are further relocated by the VARPRO procedure. The whole calculation takes 33" in a high end PC. The solution and error are displayed in Figure 3. A more inexpensive alternative would be to use the linear procedure of Section 3.1.

Figure 3 (a) L-shape problem: solution and (b) L-shape problem: error



Driscoll and Heryudono report good results for their iterative adaptation method that ends with 2100 basis functions concentrated near the singularity and comment that this is probably not an ideal method for this kind of problem. No report on the accuracy or cost of the calculation is offered.

Figure 4 Collocation points for L-shaped membrane

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